

Symbolic Methods for Automated Checking and Generation of Invariant Sets

Khalil Ghorbal

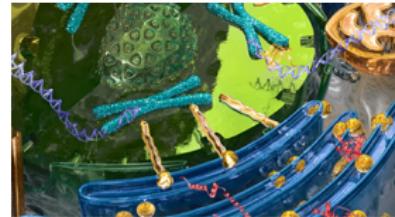
INRIA, France

Joint work with **Andrew Sogokon** and **André Platzer**

NJ, USA

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Cyber-Physical Systems



Init

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[

(

Sensing: read data from sensors

Control: actuate

Plant: evolve ◀◀◀◀◀

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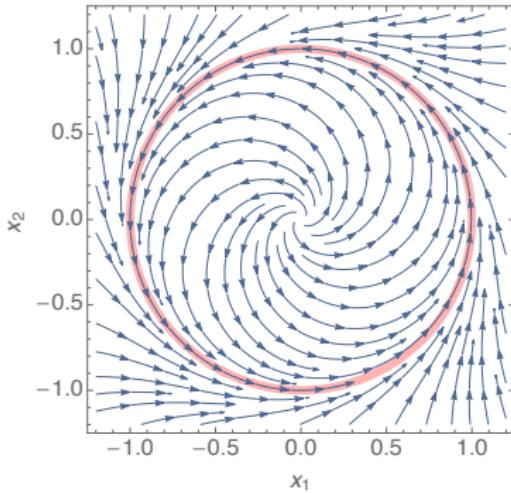
Safety

Evolution

- Continuous time
- Ordinary Differential Equations (ODE)

Qualitative Analysis of Dynamical Systems

$$(\dot{x}_1, \dot{x}_2) = (x_1 - x_1^3 - x_2 - x_1 x_2^2, x_1 + x_2 - x_1^2 x_2 - x_2^3)$$



Algebraic
Invariant
Equation

The solution for $\mathbf{x}_0 = (1, 0)$ respects $x_1(t)^2 + x_2(t)^2 - 1 = 0 \quad \forall t$

Why Are Invariants Important ?

Numerical Integration & Qualitative Analysis

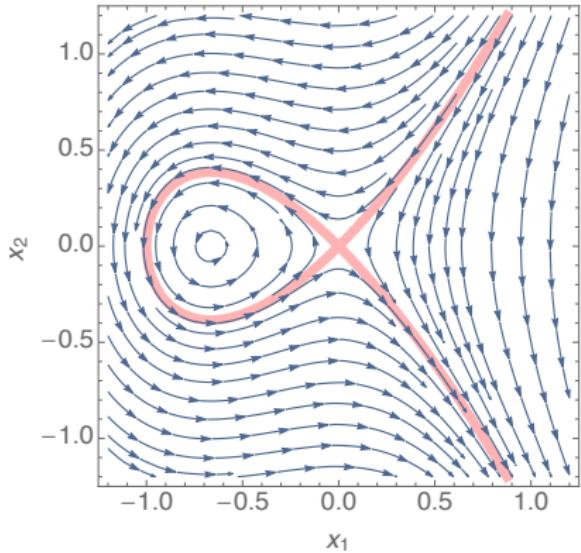
- More precise numerical integration (Geometrical Integration)
- Better understanding of the dynamics without solving the problem (some invariants represent conserved quantities like momentum or energy)

Formal Verification

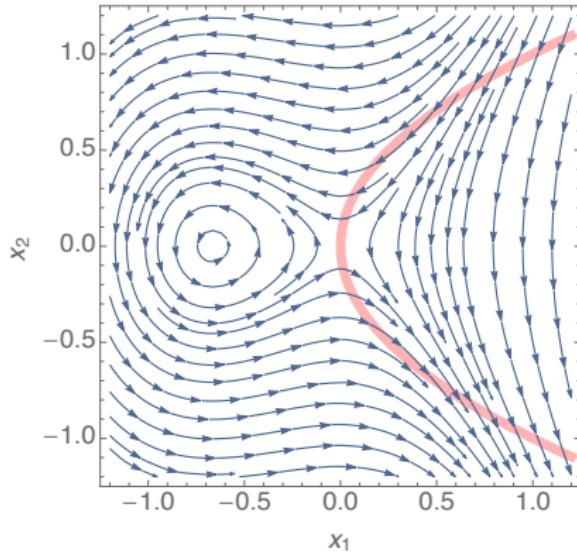
- Formal verification for dynamical and hybrid systems
- Static Analysis (as templates to statically analyze an implementation)
- Safety, Reachability, Stability

Problem I. Checking Invariance of Algebraic Equations

Given $\dot{\mathbf{x}} = (-2x_2, -2x_1 - 3x_1^2)$, $p(\mathbf{x}_0) = 0$, is $p(\mathbf{x}(t)) = 0$ for all t ?



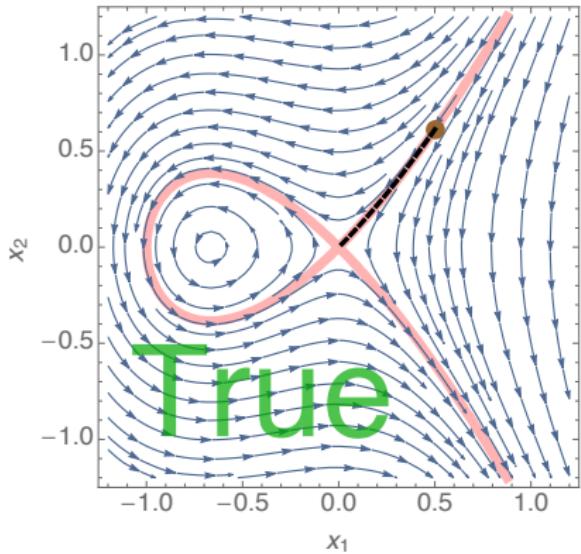
$$p(x_1, x_2) = x_1^2 + x_1^3 - x_2^2$$



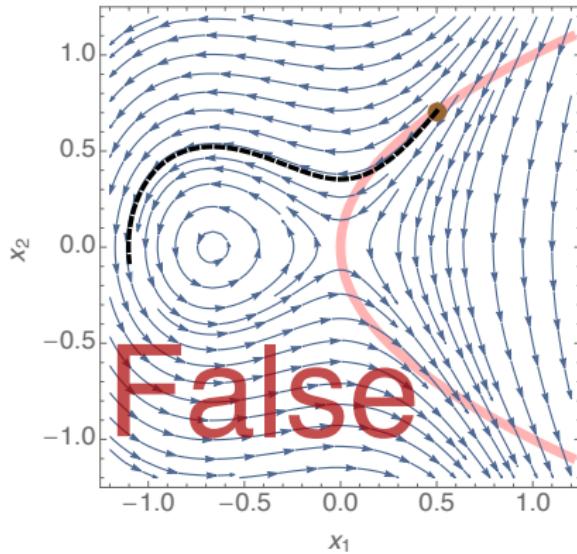
$$p(x_1, x_2) = x_1 - x_2^2$$

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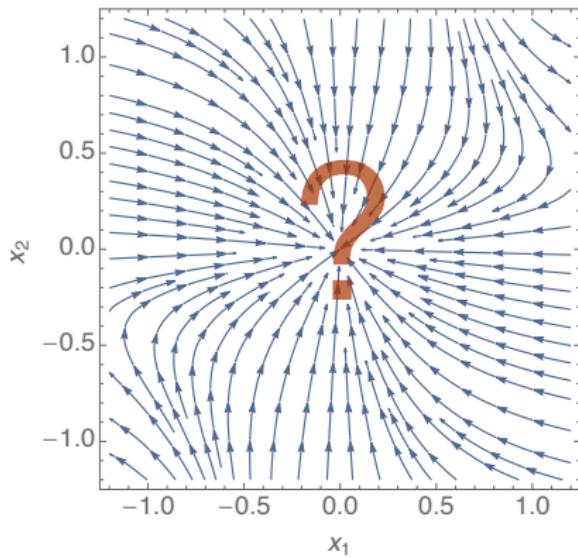
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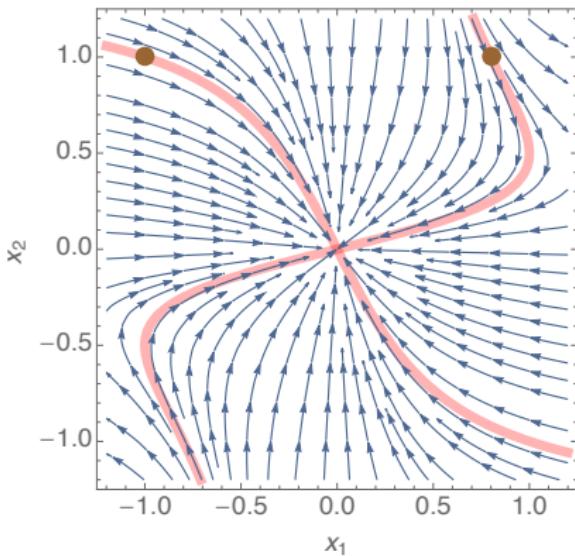
Problem II. Generate Algebraic Invariant Equations

Given $\dot{\mathbf{x}} = (-x_1 + 2x_1^2x_2, -x_2)$, how to generate p such that $p(\mathbf{x}(t)) = 0$?



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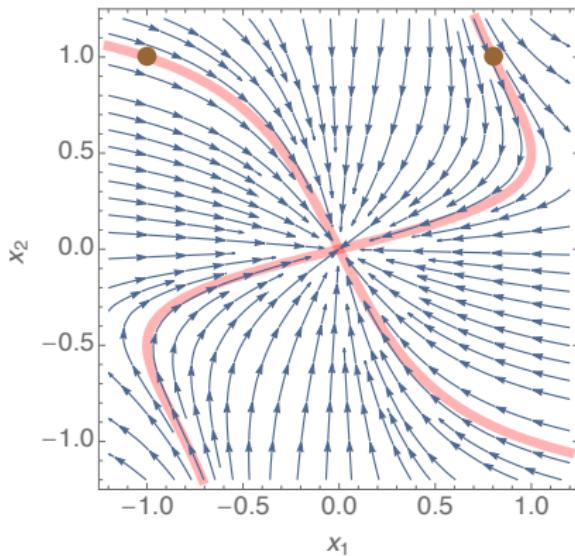
Given $\dot{\mathbf{x}} = (-x_1 + 2x_1^2x_2, -x_2)$, how to generate p such that $p(\mathbf{x}(t)) = 0$?



$$p_{(x_1(0), x_2(0))}(x_1, x_2) = (x_2(0) - x_1(0)x_2(0)^2)x_1 - x_1(0)(x_2 - x_1x_2^2) = 0$$

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$\frac{x_1}{x_2 - x_1x_2^2}$ is an invariant **rational function**.

Gradient $\nabla p := \left(\frac{\partial p}{\partial x_1}, \dots, \frac{\partial p}{\partial x_n} \right)$

Lie Derivation $\mathfrak{D}_f(p) := \frac{dp(\mathbf{x}(t))}{dt} = \langle \nabla p, \mathbf{f} \rangle \quad (\dot{\mathbf{x}} = \mathbf{f})$

Singular Locus

$$\text{SL}(p) := \{ \mathbf{x} \in \mathbb{R}^n \mid \nabla p = \mathbf{0} \} = \left\{ \mathbf{x} \in \mathbb{R}^n \mid \frac{\partial p}{\partial x_1} = 0 \wedge \dots \wedge \frac{\partial p}{\partial x_n} = 0 \right\}$$

$\mathbf{x} \in V_{\mathbb{R}}(p)$ ($p(\mathbf{x}) = 0$) is **singular** if $\mathbf{x} \in \text{SL}(p)$, **regular** otherwise.

- 1 Context
- 2 The Checking Problem
- 3 The Generation Problem
- 4 Future Avenues

Notation for “ $S \subseteq \mathbb{R}^n$ is invariant for \mathbf{f} ”

$$S \rightarrow [\dot{\mathbf{x}} = \mathbf{f}]S$$

\equiv

The set S is an invariant set for \mathbf{f}

\equiv

Starting with \mathbf{x}_0 s.t $\mathbf{x}_0 \in S$: for all $t > 0$, $\mathbf{x}(t)$ solution of the IVP $(\dot{\mathbf{x}} = \mathbf{f}, \mathbf{x}(0) = \mathbf{x}_0)$ is in S

N.B. Treating $\dot{\mathbf{x}} = \mathbf{f}$ as a program, one can think of the top formula as representing the Hoare triple $\{S\} \dot{\mathbf{x}} = \mathbf{f} \{S\}$.

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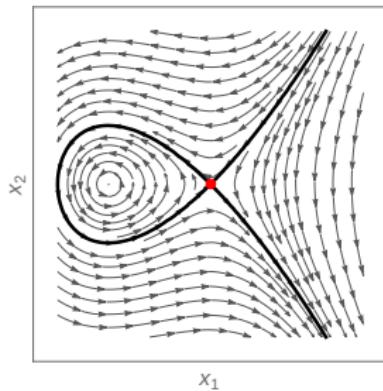
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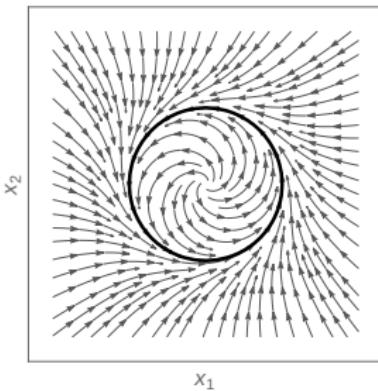
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Necessary and sufficient for smooth invariant manifolds (Lie, 1893).

$$(\text{Lie}) \frac{p = 0 \rightarrow (\mathfrak{D}_f(p) = 0 \wedge \nabla p \neq \mathbf{0})}{(p = 0) \rightarrow [\dot{x} = f] (p = 0)}$$



$p = 0$ non-smooth \times



$p = 0$ smooth ✓

Handling certain **singularities** (points where $\nabla p = \mathbf{0}$)

No flow in the problem variables at singularities on the variety

$$(\text{Lie}^\circ) \frac{p = 0 \rightarrow (\mathfrak{D}_f(p) = 0 \wedge (\nabla p = \mathbf{0} \rightarrow f = \mathbf{0}))}{(p = 0) \rightarrow [\dot{x} = f] \ (p = 0)}$$

Flow at singularities on the variety is directed into the variety

$$(\text{Lie}^*) \frac{p = 0 \rightarrow (\mathfrak{D}_f(p) = 0 \wedge (\nabla p = \mathbf{0} \rightarrow p(x + \lambda f) = 0))}{(p = 0) \rightarrow [\dot{x} = f] \ (p = 0)} .$$

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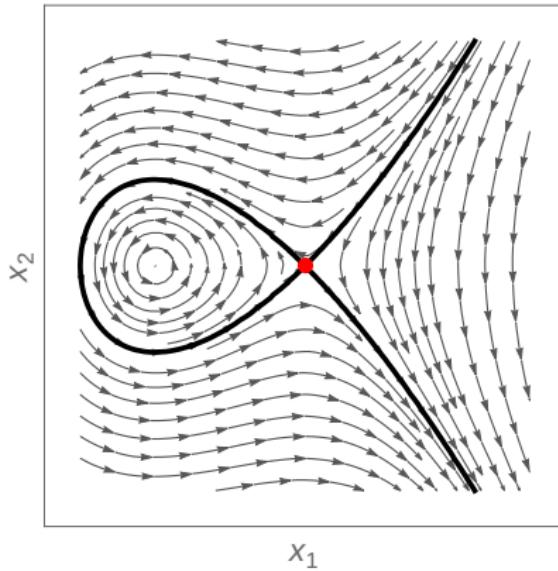
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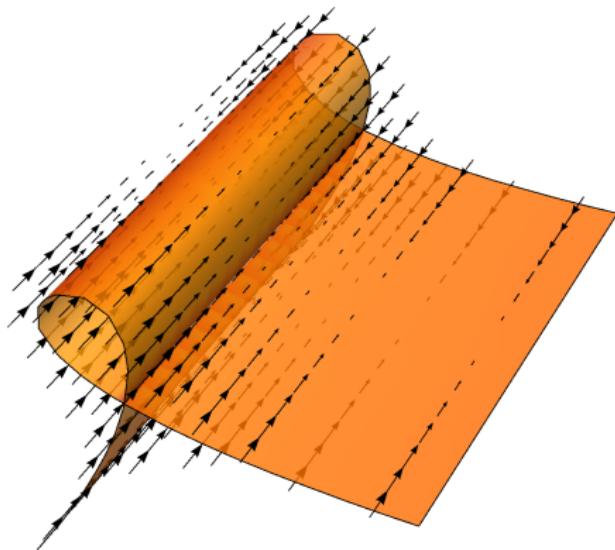
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Handling certain **singularities** (points where $\nabla p = \mathbf{0}$)



Lie **X** Lie[°] ✓ Lie* ✓

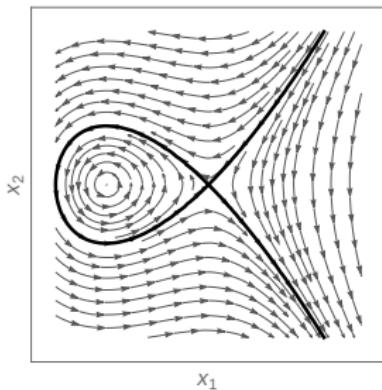
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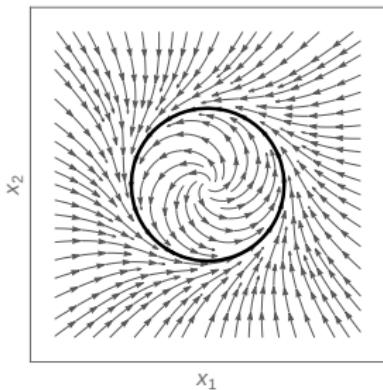
Lie **X** Lie^o **X** Lie* **✓**

Necessary and sufficient for conserved quantities (integrals of motion).

$$(FI) \frac{\mathfrak{D}_f(p) = 0}{(p = 0) \rightarrow [\dot{x} = f] \ (p = 0)}$$



p conserved ✓



p not conserved X

Continuous consecutions (C-c) and **polynomial consecutions** (P-c) are Darboux polynomials (Darboux, 1878).

$$(C\text{-c}) \frac{\exists \lambda \in \mathbb{R}, \mathcal{D}_f(p) = \lambda p}{(p=0) \rightarrow [\dot{x} = f] (p=0)},$$

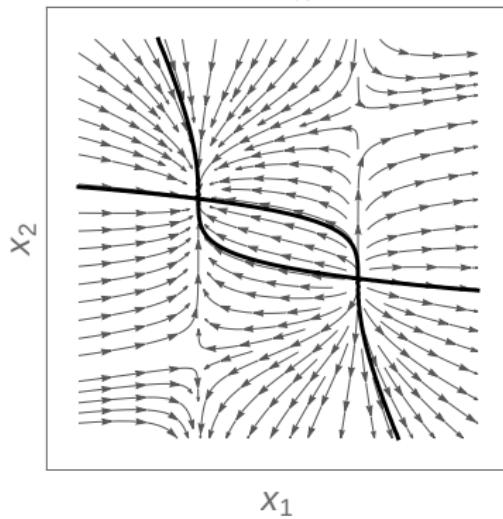
$$(P\text{-c}) \frac{\exists \lambda \in \mathbb{R}[x], \mathcal{D}_f(p) = \lambda p}{(p=0) \rightarrow [\dot{x} = f] (p=0)} .$$

Extensions of FI

[Sankaranarayanan et al., FMSD 2008]

$$\mathbf{f} = (3(x_1^2 - 4), -x_2^2 + x_1x_2 + 3), \quad p = x_2^4 + 2x_1x_2^3 + 6x_2^2 + 2x_1x_2 + x_1^2 + 3,$$

$$\mathfrak{D}_{\mathbf{f}}(p) = \underbrace{(6x_1 - 4x_2)}_{\lambda} p$$



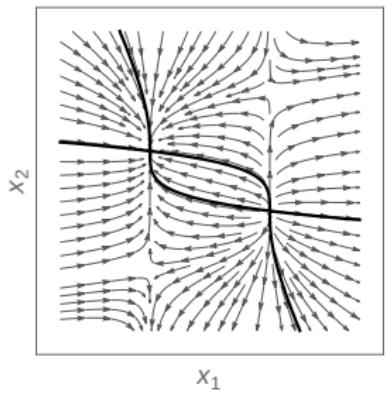
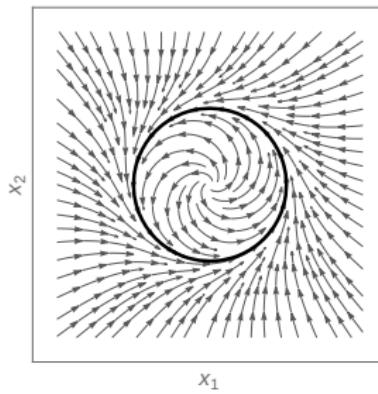
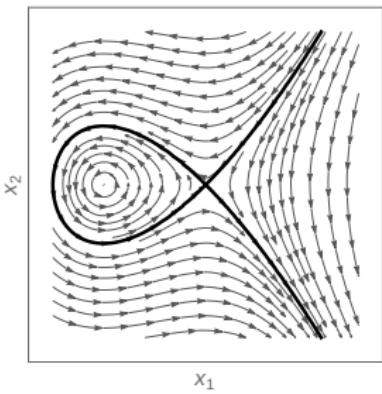
FI X C-c X P-c ✓

Differential Radical Invariants (DRI)

[G. et al., TACAS 2014, SAS 2014]

Necessary and sufficient for invariant varieties.

$$(DRI) \frac{p = 0 \rightarrow \bigwedge_{i=0}^{N-1} \mathfrak{D}_f^{(i)}(p) = 0}{(p = 0) \rightarrow [\dot{x} = f] \ (p = 0)}$$

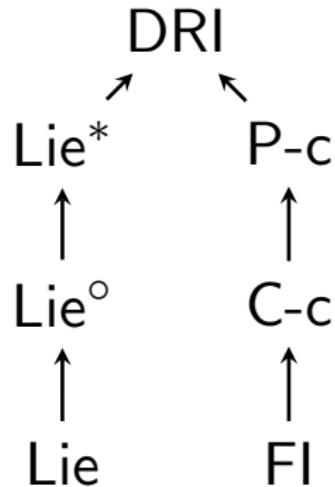


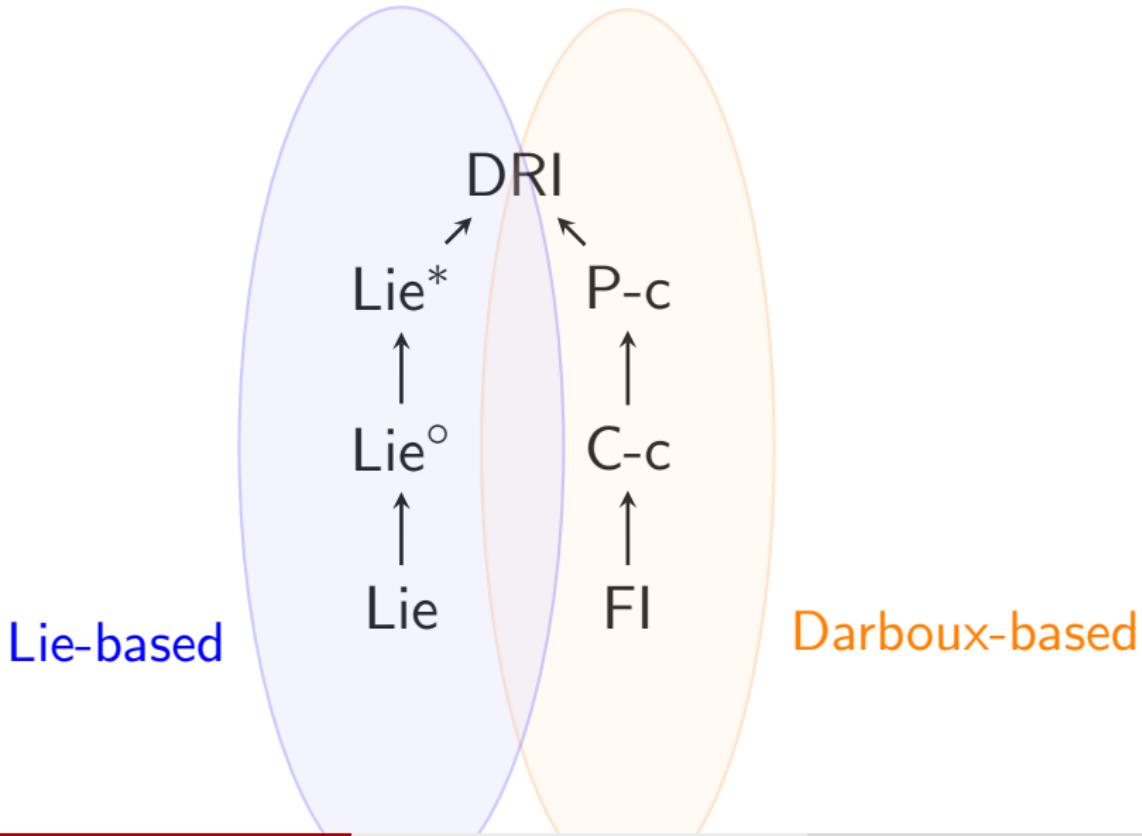
$$(R_A) \frac{A}{S_A : T_A \longrightarrow [\dot{x} = f] S_A : T_A} \quad (R_B) \frac{B}{S_B : T_B \longrightarrow [\dot{x} = f] S_B : T_B}$$

Partial Order

$R_A \preccurlyeq R_B$ if and only if $A \implies B$ and T_A is a “subtype” of T_B .

- $R_A \sim R_B$ ($R_A \preccurlyeq R_B$ and $R_A \succcurlyeq R_B$) **Equivalence.**
- $R_A \prec R_B$ ($R_A \preccurlyeq R_B$ and $R_A \not\succcurlyeq R_B$) **Strict increase** of deductive power





Square-free reduction of a polynomial

$$h = h_1^{\alpha_1} h_2^{\alpha_2} \cdots h_k^{\alpha_k}$$

Geometrically $V_{\mathbb{R}}(h) \equiv_{\mathbb{R}} V_{\mathbb{R}}(\text{SF}(h))$.

- SF **automated pre-processing** step in **computer algebra** systems
- Is it a “good idea” to apply SF for invariance checking ?

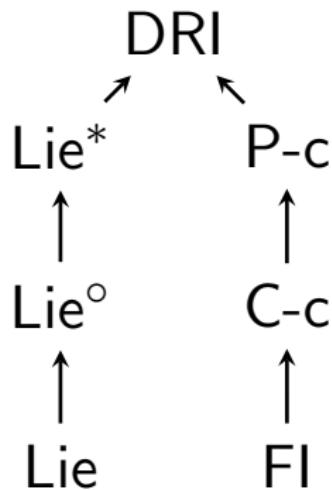
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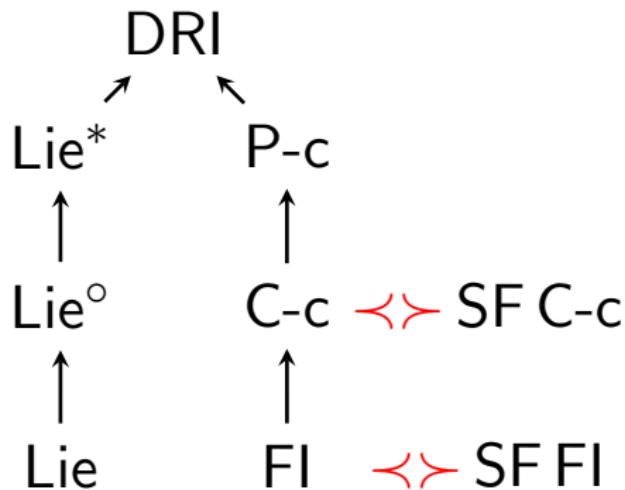
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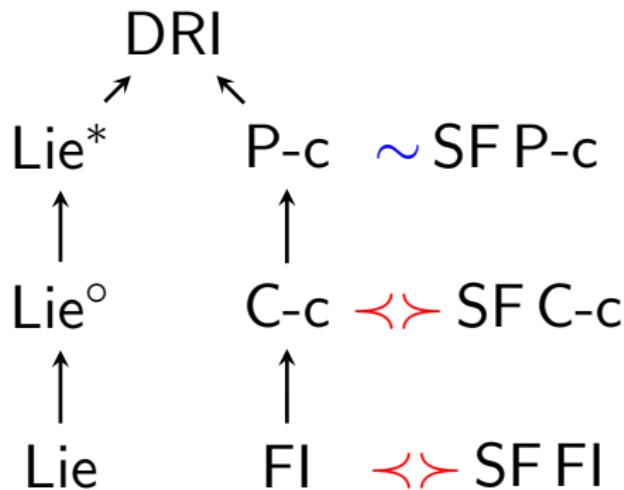
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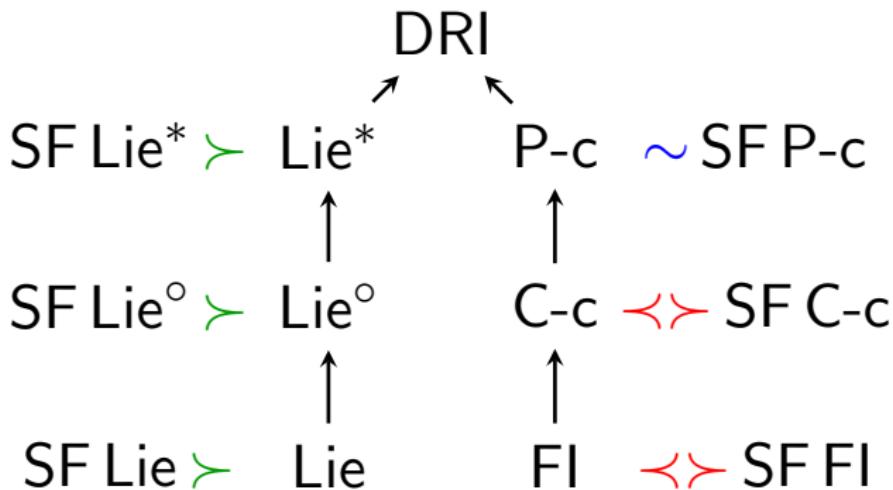
Square-free Reduction

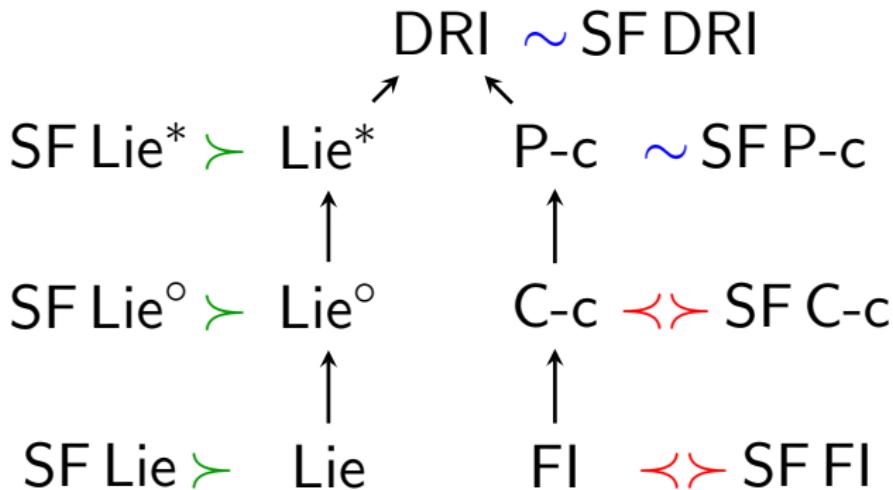


Square-free Reduction









So far we have only seen **algebraic** sets: $p = 0$

- For $\wedge_i p_i = 0$, we can rewrite using $\sum_i p_i^2 = 0$
- We can do better [SAS'14]

What about **semi-algebraic** sets:

- Sets of the form $p \leq 0$
- Closed Sets
- Arbitrary Sets: boolean formulae with polynomial equalities and inequalities

Sub-tangent Vector

A vector $\mathbf{v} \in \mathbb{R}^n$ is sub-tangential to a set $S \subseteq \mathbb{R}^n$ at $\mathbf{x} \in S$ if

$$\liminf_{\lambda \rightarrow 0^+} \frac{\text{dist}(S, \mathbf{x} + \lambda \mathbf{v})}{\lambda} = 0. \quad (\text{dist}(S, \mathbf{x}) \equiv \inf_{\mathbf{y} \in S} \|\mathbf{x} - \mathbf{y}\|_1)$$

Contingent Cone

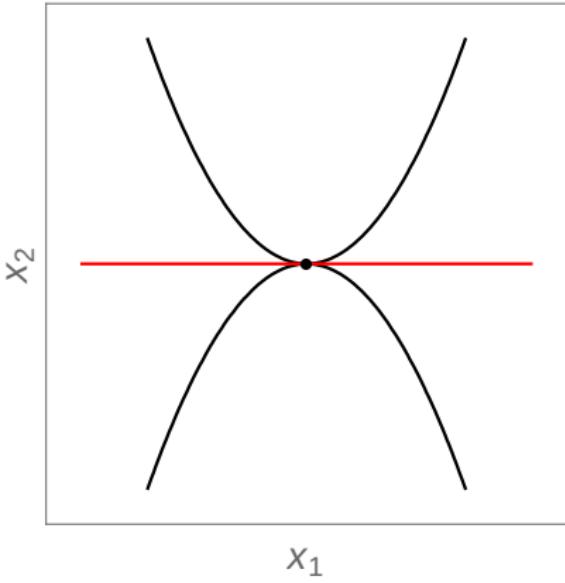
$K_{\mathbf{x}}(S)$: the set of all sub-tangent vectors to a set S at $\mathbf{x} \in S$.

Nagumo's Theorem

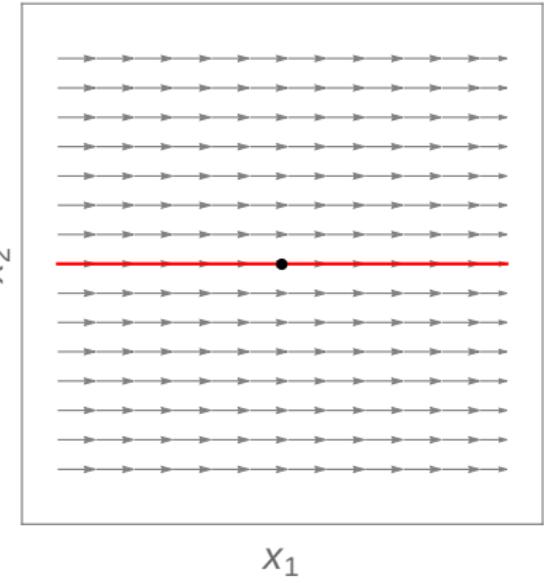
A **closed** set $S \subset \mathbb{R}^n$ is **positively invariant** under the flow of the system if and only if $\mathbf{f}(\mathbf{x}) \in K_{\mathbf{x}}(S)$ for all $\mathbf{x} \in \text{bdr}(S)$ (boundary of S).

Contingent Cone of Boolean Formulae

$$K_x(S_1) \cap K_x(S_2) \supset K_x(S_1 \cap S_2)$$



$$x_2 + x_1^2 = 0 \wedge x_2 - x_1^2 = 0$$



$$\dot{x}_1 = 1, \dot{x}_2 = 0$$

(Non-strict) Barrier Certificate ✓

$(\forall \mathbf{x} \in \mathbb{R}^n, \mathfrak{D}_f(p) \leq 0) \rightarrow p \leq 0$ is a positive invariant

Unsound Barrier Certificate ✗

$(\forall \mathbf{x} \text{ s.t. } \mathbf{p}(\mathbf{x}) = \mathbf{0}, \mathfrak{D}_f(p) \leq 0) \rightarrow p \leq 0$ is a positive invariant

Strict Barrier Certificate ✓

$(\forall \mathbf{x} \text{ s.t. } p(\mathbf{x}) = 0, \mathfrak{D}_f(\mathbf{p}) < \mathbf{0}) \rightarrow p \leq 0$ is a positive invariant

Differential Invariants (DI)

$$(DI) \frac{D(S)_{\dot{x}}^f}{S \rightarrow [\dot{x} = f] S},$$

$D(S)_{\dot{x}}^f$: substitute each \dot{x}_i in $D(S)$ with $f_i(x)$

$$D(r) = 0 \quad \text{for numbers,}$$

$$D(x) = \dot{x} \quad \text{for variables,}$$

$$D(a + b) = D(a) + D(b),$$

$$D(a \cdot b) = D(a) \cdot b + a \cdot D(b),$$

$$D(a \leq b) \equiv D(a) \leq D(b), \quad \text{accordingly for } \geq, >, < . \quad (\mathbf{BC})$$

$$D(S_1 \wedge S_2) \equiv D(S_1) \wedge D(S_2),$$

$$D(S_1 \vee S_2) \equiv D(S_1) \wedge D(S_2), \quad (\wedge \text{ here is important for soundness})$$

Non-smooth Strict Barrier Certificate (NSSBC)

Apply Strict Barrier Certificate on Active Boundaries

$$\text{(NSSBC)} \frac{\left(\min_{i=1,\dots,k} \max_{j=1,\dots,m(i)} p_{ij} = 0 \right) \rightarrow \mathfrak{D}_f \left(\min_{i=1,\dots,k} \max_{j=1,\dots,m(i)} p_{ij} \right) < 0}{\left(\bigvee_{i=1}^k \bigwedge_{j=1}^{m(i)} p_{ij} \leq 0 \right) \rightarrow [\dot{x} = f] \left(\bigvee_{i=1}^k \bigwedge_{j=1}^{m(i)} p_{ij} \leq 0 \right)}.$$

Check Invariance of $p_1 \leq 0 \vee p_2 \leq 0$

NSSBC

DI

$$\begin{aligned} & (p_1 < p_2 \wedge p_1 = 0 \rightarrow \mathfrak{D}_f(p_1) < 0) \\ \wedge \quad & (p_1 > p_2 \wedge p_2 = 0 \rightarrow \mathfrak{D}_f(p_2) < 0) \quad \mathfrak{D}_f(p_1) \leq 0 \wedge \mathfrak{D}_f(p_2) \leq 0 \\ \wedge \quad & (p_1 = p_2 = 0 \rightarrow \mathfrak{D}_f(p_1) < 0 \vee \mathfrak{D}_f(p_2) < 0) \end{aligned}$$

Definitions

$$\begin{aligned}\text{In}_f(S) &\equiv \{\mathbf{x} \in \mathbb{R}^n \mid \exists \epsilon > 0. \forall t \in (0, \epsilon). \mathbf{x}(t) \in S\}, \\ \text{In}_{(-f)}(S) &\equiv \{\mathbf{x} \in \mathbb{R}^n \mid \exists \epsilon > 0. \forall t \in (0, \epsilon). \mathbf{x}(-t) \in S\},\end{aligned}$$

Characterization

An arbitrary set $S \subset \mathbb{R}^n$ is a positive invariant for \mathbf{f} if and only if

$$S \subseteq \text{In}_f(S) \text{ and } S^c \subseteq \text{In}_{(-f)}(S^c)$$

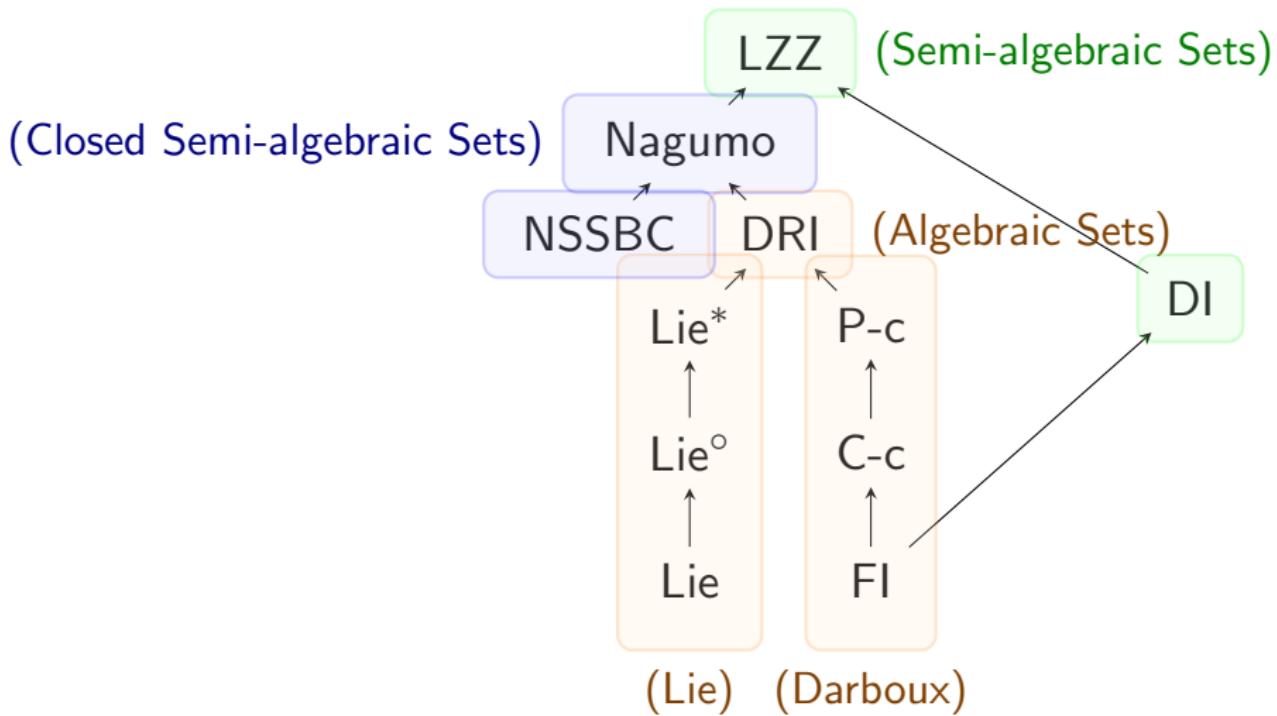
or equivalently

$$\text{In}_{(-f)}(S) \subseteq S \subseteq \text{In}_f(S)$$

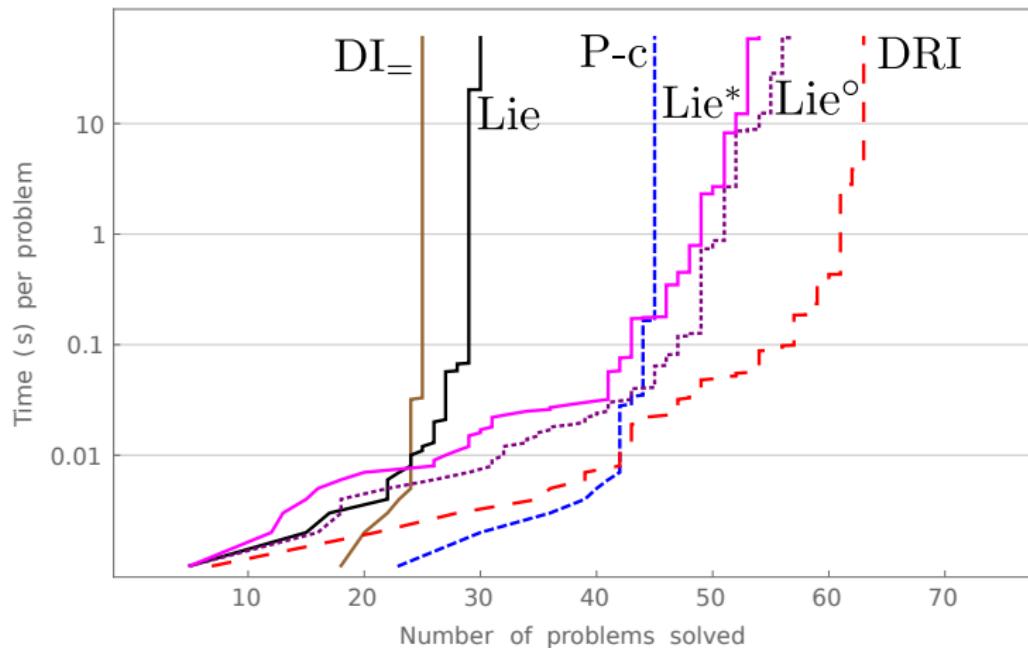
- $\text{In}_f(S)$ can be computed using high-order Lie derivatives !

Overview

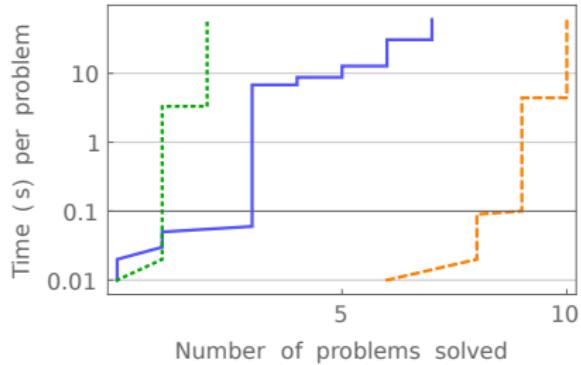
Proof Rules for Checking Invariance of Semi-algebraic Sets



Experimental Performance: Algebraic Sets

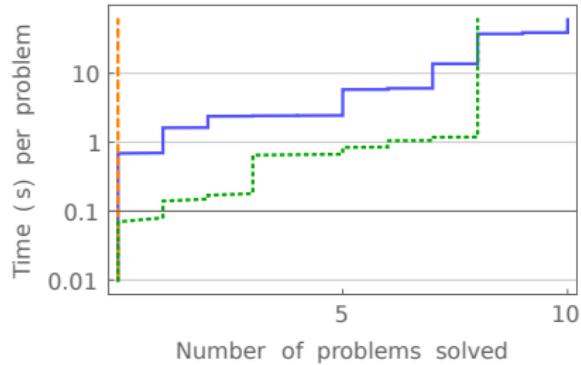


Experimental Performance: Semi-algebraic Sets



LZZ vs DI

— LZZ - - - DI - · - NSSBC



LZZ vs NSSBC

- 1 Context
- 2 The Checking Problem
- 3 The Generation Problem
- 4 Future Avenues

Template-Based

- Fix a template: generic polynomials with symbolic coefficients
- Use sufficient conditions to derive constraints over the coefficients
- Solve the system
- In practice:
 - templates of the form $p = 0$ (algebraic sets) with Darboux condition ($\mathfrak{D}_f(p) \in \langle p \rangle$) work for $n \leq 10$ and $d \leq 3$.
 - templates of the form $p \leq 0$ relying on Barrier Certificates (SOSTools)

Discrete Abstraction

- Discrete the space with the signs of a given set of polynomials
- Relies on sufficient conditions to remove spurious transitions
- Issue: How to populate and eventually refine the initial set of polynomials

Matrix Representation: Intuition

Suppose we have a 2-dimensional ODE $(\dot{x}_1, \dot{x}_2) = (x_1, x_2)$

Matrix Representation: Intuition

Suppose we have a 2-dimensional ODE $(\dot{x}_1, \dot{x}_2) = (x_1, x_2)$

- ① Start with parametric h of degree 1: $h = \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3$

Matrix Representation: Intuition

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$$h = x_2(0)x_1 - x_1(0)x_2$$

- 1 Context
- 2 The Checking Problem
- 3 The Generation Problem
- 4 Future Avenues

Challenges

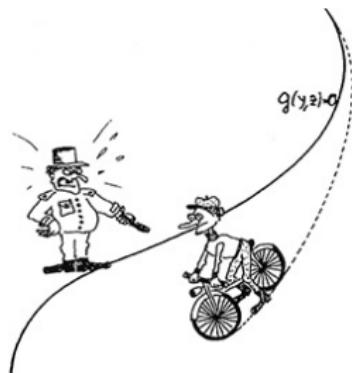


Differential-Algebraic Equations (DAE)

- Verification and Faithful Simulation for cyber-physical systems with DAE

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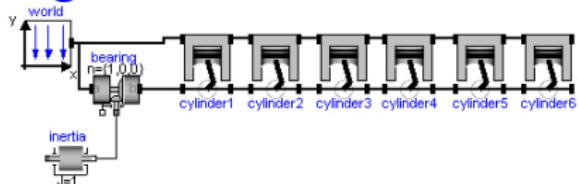
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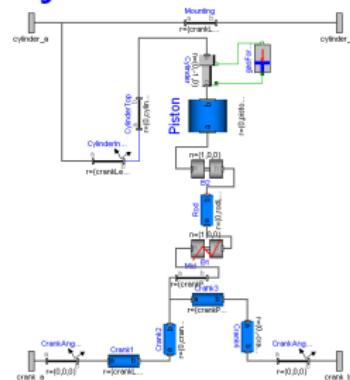
- $\mathbf{0} = \mathbf{F}(\mathbf{x}, \dot{\mathbf{x}}, t)$
- $$\begin{cases} \dot{\mathbf{x}} = \mathbf{f}(\mathbf{y}, \mathbf{x}) \\ \mathbf{0} = \mathbf{g}(\mathbf{y}, \mathbf{x}) \end{cases}$$
- Compositional design
- Tools: Dymola (Dassault Systèmes), Modelica

V6 Engine Simple Combustion Model (Modelica)

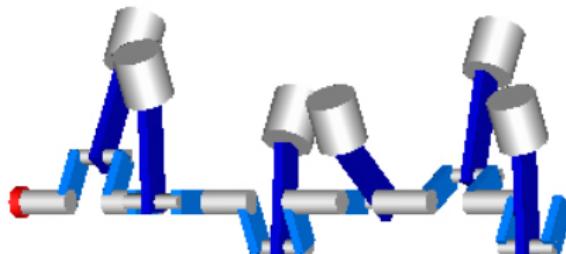
Engine



Cylinder



Simulation



Combining Static Analysis and Symbolic Computation

Invariants Generation for DAE

- Extends previous work (algebraic approach)
- Semi-explicit form of index 1 (specific class of DAE)

Hybrid Simulation is Hard

- Well-founded operational semantics (compilation, index reduction)
 - Preserve compositionality in presence of mode changes
 - Proper handling of zero-crossing
(detection and consistent initialization)
 - Cascades of zero-crossings (sliding modes)
- ➡ Investigate the use of **static analysis** and **symbolic computation**

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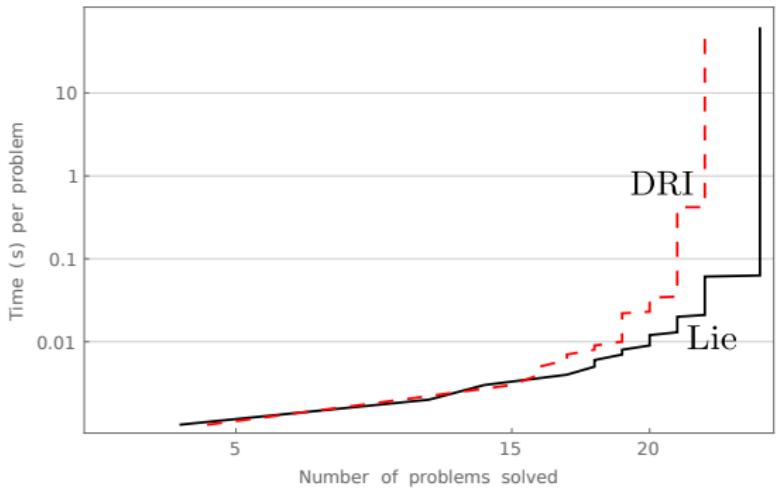
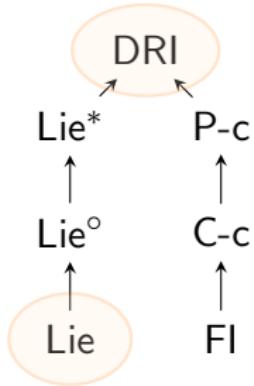
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Thanks for your attention !



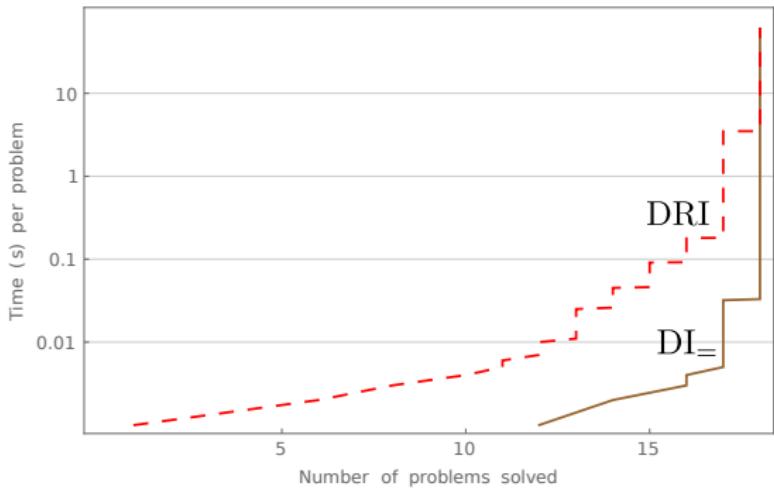
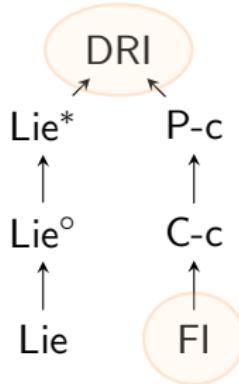
Smooth invariant manifolds (Lie vs DRI)

Lie and DRI decide invariance for **smooth invariant manifolds**.



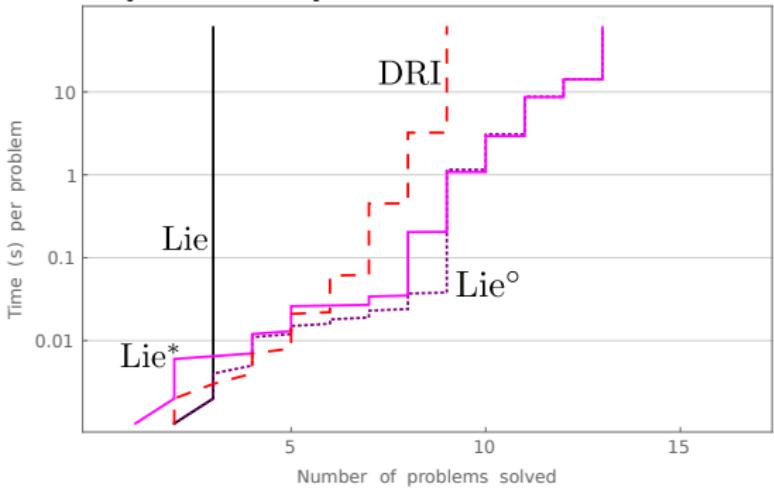
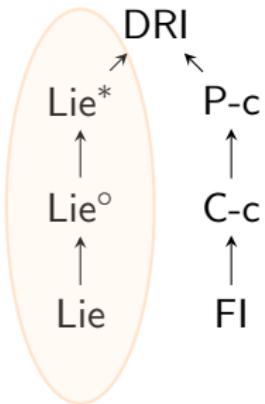
Functional invariants (DI vs DRI)

DI_\equiv and DRI decide invariance of varieties of **conserved quantities**.



Singularities at Equilibria (Lie, Lie° & Lie^* vs DRI)

Lie° , Lie^* and DRI decide invariance for varieties of with **singularities that are equilibrium points**.



$$\begin{aligned} & (h_1 > \max(h_2, \dots, h_m) \rightarrow \mathcal{D}_f(h_1) < 0) \\ \wedge \quad & (h_1 < \max(h_2, \dots, h_m) \rightarrow \mathcal{D}_f(\max(h_2, \dots, h_m)) < 0) \\ \wedge \quad & (h_1 = \max(h_2, \dots, h_m) \rightarrow \mathcal{D}_f(h_1) < 0 \wedge \mathcal{D}_f(\max(h_2, \dots, h_m)) < 0) \end{aligned}$$

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